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Title: Eulerian Applications Project - xRage The xRage Equation of State: Supported EOS Models

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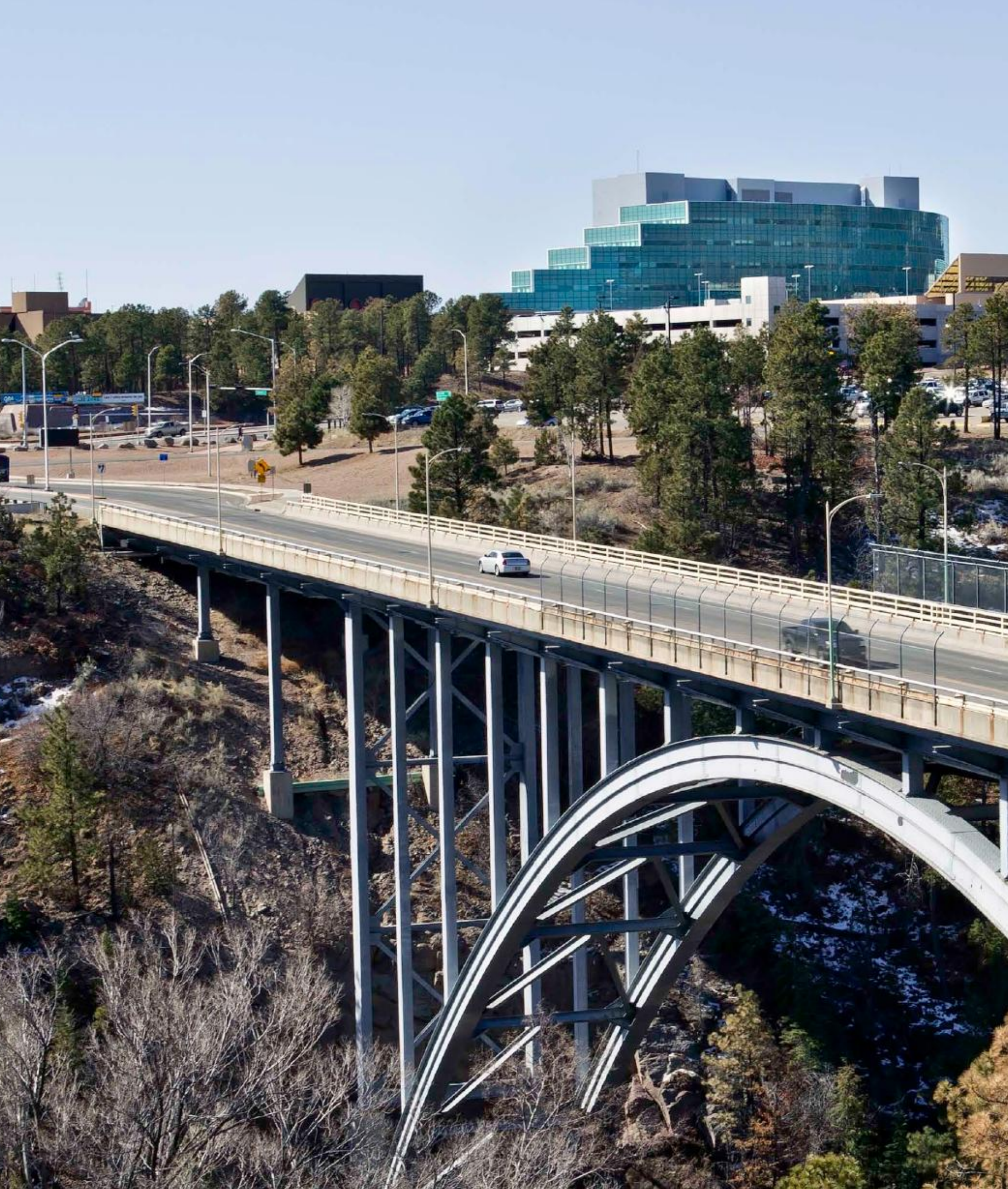

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Eulerian Applications Project - xRage

The xRage Equation of State: Supported EOS Models

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CCS-2

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Supported EOS Models

- The equation of state model to be used in setting up a pressure-temperature table is specified by the input parameter eostype
- Unless stated otherwise the standard cgs+eV units for xRage are used
- density – grams/cc, specific volume cc/gram
- pressure – microbar
- specific internal energy – ergs/gram
- temperature – eV/k
- Specific heats – ergs/gram/(eV/k)
- What a specific model uses a different unit set for input it will be explicitly stated
- Quantities such are the Grüneisen exponents are dimensionless
- Note: In this unit set pressures and specific internal energies on the order of millions and above are normal.

Analytic Mixture Models

Perfect Gas Motivated EOS Models

- This class of models is selected by the following values for the input parameter **keos**
  - **keos** = 0 - mixture of perfect gases
  - **keos** = -1 – Mixture of stiff perfect gases – inconsistent temperature
  - **keos** = -2 – stiff mixtures with crush curve – inconsistent temperature
  - **keos** = -3 – radiation mix, just used for debugging
  - **keos** = -4 – stiff mixtures – positive pressure – inconsistent temperature
  - **keos** = -5 – stiff mixture with ghosts – inconsistent temperature
  - **keos** = -6 – stiff mixture – thermodynamically consistent temperature

keos = 0 – Perfect gas mixture

- Formula: $P = \Gamma\rho e, e = C_V T$
- Input:
  - **keos** = 0
  - **nummat** = N
  - **matdef**(16,mat) = Grüneisen exponent Γ for material m
  - **matdef**(30,mat) = Specific Heat at constant volume C_V for material m
- Mixture solution: given a specific internal energy e and specific volume V for the mixture together with the component mass fractions $\mu_k, k = 1, \ldots, N$, the pressure and temperature of the mixture are given by

$$e = \sum_{k=1}^{N} \mu_k e_k = \sum_{k=1}^{N} \mu_k C_{V,k} T = C_V$$

$$PV = \sum_{k=1}^{N} \mu_k \Gamma_k C_{V,k} T = \Gamma e, \Gamma = \frac{\sum_{k=1}^{N} \mu_k \Gamma_k C_{V,k}}{C_V}$$

keos = -1,-4,-5

- Model: $e = C_V(T - T_0), \frac{(P+\kappa)}{\rho} = \frac{\kappa}{\rho_0} + \Gamma e$
  - Let $\kappa = (\Gamma + 1)P_\infty$, $e_\infty = \frac{\kappa}{\Gamma\rho_0}$ then $(P + (\Gamma + 1)P_\infty) = \Gamma(e + e_\infty)\rho$
- Input: (numat as for **keos**=0)
  - **matdef**(3,mat) = κ for material mat
  - **matdef**(16,mat) = Γ for material mat
  - **matdef**(21,mat) = ρ_0 for material mat
  - **matdef**(26,mat) = T_0 for material mat
  - **matdef**(30,mat) = C_V for material mat
  - **p_stiff** (0) – extrapolate EOS below p_stiff
- Mixture: Solve the system for temperature and pressure
  - $e = \sum_{k=1}^{N} \mu_k C_{V,k}\left(T - T_{0,k}\right)$
  - $V = \frac{1}{\rho} = \sum_{k=1}^{N} \mu_k \frac{\frac{\kappa_k}{\rho_{0,k}} + \Gamma_k C_{V,k}\left(T - T_{0,k}\right)}{P + \kappa_k}$, this is a rational equation in *P*
- These variations of the stiff gamma law model generally will not return negative pressures unless the user enters a negative value for the input variable p_stiff in their input file.

keos = -2

- This model uses an undocumented pore crush model and probably should be removed from xRage
- Input:
  - **matdef**(3,mat) = κ for material mat
  - **matdef**(16,mat) = Γ for material mat
  - **matdef**(21,mat) = ρ_0 for material mat
  - **matdef**(22,mat) = ρ_{amb} ambient density for the crush model
  - **matdef**(23,mat) = P_e ramp start pressure
  - **matdef**(24,mat) = P_c ramp crush pressure
  - **matdef**(25,mat) = $\frac{dP_e}{d\rho}$ a slope associated with the crush ramp
  - **matdef**(26,mat) = T_0 for material mat
  - **matdef**(30,mat) = C_V for material mat
- Since the model is undocumented it is not possible to provide guidance on appropriate values for these parameters
- This model may have never been used, at least in recent memory

keos = -6

- Thermodynamically Consistent Stiff Gamma Law equation of state

$$P + (\Gamma + 1)P_\infty = \frac{\Gamma}{V}(e + e_\infty), \qquad e + e_\infty = C_V T + P_\infty V$$

- Helmholtz free energy

$$F + F_\infty = C_V(T - T_\infty) - \mathrm{T}C_V \log\left[\frac{T}{T_\infty}\left(\frac{V}{V_\infty}\right)^{\Gamma}\right] + P_\infty(V - V_\infty) - S_\infty(T - T_\infty)$$

- We note that this free energy is just the Helmholtz free energy for a perfect gas with an added linear term in specific volume and temperature
- Input
  - **matdef**(3,mat) = P_∞, **matdef**(10,mat) = e_∞ , **matdef**(16,mat) = Γ
  - **matdef**(21,mat) = V_∞, **matdef**(30,mat) = C_V
  - The other parameters are not used in the implemented model and may be taken as zero which is also the default value for e_∞
- The domain is $P > -P_\infty$, for mixtures the domain is $P > -\min P_{\infty,mat}$
- The pressure temperate equilibrium solution solves a rational equation in pressure, which has a unique solution in the mixture domain

Models for Use with P-T Tabular EOS
keos=3

Supported EOS Models
Sesame – eostype(mat) = 0 or 99

- Sesame
  - eostype(mat) = 0 - xRage intrinsic Sesame support
  - eostype(mat) = 99 – Sesame suport via EOSPAC
  - matid(mat) = Sesame material id to be used

Supported EOS Models
JWL – eostype(mat) = 1

$$P = P_r(V) + \frac{w}{V}\left(E - E_r(V)\right), E = E_r(V) + C_V T$$

$$P_r(V) = Ae^{-R_1 \frac{V}{V_0}} + Be^{-R_2 \frac{V}{V0}}, E_r(V) = \frac{AV_0}{R_1} e^{-R_1 \frac{V}{V_0}} + \frac{BV_0}{R_2} e^{-R_2 \frac{V}{V0}}$$

– A = matdef(3,mat), B = matdef(4,mat)

– R_1= matdef(10,mat), R_2=matdef(11,mat)

– w = matdef(16,mat), $\rho_0 = {}^{1}/_{V_0}$= matdef(21,m), C_V = matdef(30,mat)

Supported EOS Models
eostype(mat) = 2 – Polynomial Equation of State

$$P = \begin{cases} (\kappa_a + (\kappa_b + \kappa_c\mu)\mu)\mu + \Gamma\rho E & \mu > 0 \\ \kappa_a\mu + \Gamma\rho E & \mu \le 0 \end{cases}, \quad \mu = \frac{\rho}{\rho_0} - 1$$

$$e = C_V(T - T_0 + P_0/(\Gamma\rho_0 C_V))$$

- κ_a= matdef(3,mat), κ_b= matdef(10,mat), κ_c = matdef(11,mat)
  - the above have units of pressure
- Γ= matdef(16,mat), ρ_0 = matdef(21,mat)
- T_0 = matdef(26,mat), P_0 = matdef(28,mat), C_V = matdef(30,mat)

Supported EOS Models
eostype(m) = 3 , Steinberg-Mie-Grüneisen

$$P = \begin{cases} \dfrac{\rho_0 c_0^2 \mu \left[1 + \left(1 - \frac{\Gamma_0}{2}\right)\mu - \frac{b}{2}\mu^2\right]}{\left[1 - (s_1 - 1)\mu - s_2 \frac{\mu^2}{1+\mu} - s_3 \frac{\mu^3}{(1+\mu)^2}\right]^2} + (\Gamma_0 + b\mu)\rho E \;, & \rho \geq \rho_0 \\ \rho_0 c_0^2 \mu + \Gamma_0 \rho E \;, & \rho < \rho_0 \end{cases}$$

$$\mu = \frac{\rho}{\rho_0} - 1$$

$$E = C_V (T - T_0)$$

- c_0= matdef(3,m), Γ_0 = matdef(16,m), b = matdef(17,m), s_1 = matdef(4,m), s_2 = matdef(10,m), s_3 = matdef(11,m)
- ρ_0 = matdef(21,m), T_0 = matdef(26,m), P_0 = matdef(28,m) ignored, C_V = matdef(30,mat)
- Note: the formula for P is based on a misinterpretation of the formula in Steinberg's report. In the reference the quantity E is energy per reference volume not energy per volume. Consequently the above formula for *P* does not give the correct Hugoniot. The second inconsistency is the specific internal energy temperature relation of which the above formula is only the linearization of the thermodynamically consistent equation near the reference values. If matdef(2,m) is non-zero, then the inconsistencies in the specific heat and specific internal energy are corrected and the value of matdef(30,m) specifies the reference density times the specific heat at constant volume $\rho_0\ C_V$= matdef(30,m), and the incomplete EOS becomes

$$P = \begin{cases} \dfrac{\rho_0 c_0^2 \mu \left[1 + \left(1 - \frac{\Gamma_0}{2}\right)\mu - \frac{b}{2}\mu^2\right]}{\left[1 - (s_1 - 1)\mu - s_2 \frac{\mu^2}{1+\mu} - s_3 \frac{\mu^3}{(1+\mu)^2}\right]^2} + (\Gamma_0 + b\mu)\rho_0 E \;, & \rho \geq \rho_0 \\ \rho_0 c_0^2 \mu + \Gamma_0 \rho E \;, & \rho < \rho_0 \end{cases}$$

Supported EOS Models
eostype(m) = 4 The Nadyozhin Equation of State

- Reference: D. K. Nadyozhin and A. V. Yudin, *Equation of state under nuclear statistical equilibrium conditions*, Astronomy Letters, **30**, no. 9, 634-646, 2004
- equation of state for completely ionized matter, electron & positron component --- fermi-dirac statistics using various asymptotic expansions where possible
  ion component --- a perfect gas approximation
  black-body radiation
- $\bar{a}$ = matdef(18,m), $y_e=\frac{\bar{z}}{\bar{a}}$ = matdef(19,m)

Supported EOS Models
eostype(m) = 5, HOM Solid

$$P - P_r(V) = \frac{\Gamma}{V}\big(E - E_r(V)\big), E = E_r(V) + C_V\big(T - T_r(V)\big)$$

$$P_r(V) = \begin{cases} P_{min} + P_r{}'(V_{max})(\rho - \rho_{\min}) & \rho < \rho_0 \\ \left[\frac{c_0}{V_0 - s(V_0 - V)}\right]^2 (V_0 - V) & \rho_0 \le \rho \le \rho_{\max} \\ P_{max} + P_r{}'(V_{min})(\rho - \rho_{\max}) & \rho_{\max} < \rho \end{cases}$$

$$E_r(V) = \frac{P_r(V) + P_0}{2}(V_0 - V)$$

$$T_r(V) = \exp[t_0 + t_1(\log V) + t_2(\log V)^2 + t_3(\log V)^3 + t_4(\log V)^4]$$

- c_0=matdef(2,m), s=matdef(3,m), t_i=matdef(7+i,m)
- Γ=matdef(12,m), C_V=matdef(13,m) (units calorie/gram/kelvin)
- $V_0 = \frac{1}{\rho_0}$ = matdef(14,m), P_0=matdef(19,m)
- P_{min}=matdef(25,m), P_{max}=matdef(26,m)
- $P_{min} = P_r(V_{max})$, $P_{max} = P_r(V_{min})$
- Note: A variation of this EOS that uses a stiff gamma law fit for expansion can be selected using eostype(m) = 55

Supported EOS Models
eostype(m) = 6, HOM Gas

$$P = P_r(V) + \frac{\Gamma(V)}{V}[E - E_r(V)], \quad E = E_r(V) + C_V[T - T_r(V)]$$

- $\log[P_r(V)] = \sum_{k=0}^{4} p_k\,[\log(V)]^k, \log[E_r(V) + z] = \sum_{k=0}^{4} e_k\,[\log(V)]^k$
  $$\log[T_r(V)] = \sum_{k=0}^{4} t_k\,[\log(V)]^k, \quad \Gamma(V) = -\frac{V}{T_r(V)}T'_r(V)$$
- p_k= matdef(2+k,m), e_k= matdef(7+k,m), t_k= matdef(12+k,m)
- C_V = matdef(17,m) – note units are input in calorie/gram/kelvin
- $z =$ matdef(18,m)
- The use of polynomials in the logarithm of the specific volume means that this model can be subject to severe domain restrictions. The internals of the HOM gas routine attempts to compute the specific volume limits and for values that fall outside these limits linear extrapolation in specific volume is used.
- Note: A variation of this EOS that uses a stiff gamma law fit for expansion can be selected using eostype(m) = 66

Supported EOS Models eostype(m) = 7, National Bureau of Standards/S-Cubed Water-ice

- Multiphase equation of state for water, including liquid, vapor, and several solid ice phases
- References:
  - Goodwin, R.D. and L.A. Weber, *Comparison of two melting-pressure equations constrained to the triple point using data for eleven gases and three metals. Technical note (final)*, COM--75-10052 NBS-TN--183. 1963.
  - Baker, J., et al., *Computational Equation of State AQUA Water*, S-CUBED. 1988.
- This is a very good equation of state for water. Applications for liquid vapor phase transition show good results.

Supported EOS Models
eostype(m) = 8, LLNL QEOS

- **New quotidian equation of state (QEOS) for hot dense matter More, R.M. ; Warren, K.H. ; Young, D.A. ; Zimmerman, G.B.** Phys. Fluids, 1988, Vol.3 1(10)
- Abstract: The quotidian equation of state (QEOS) is a general-purpose equation of state model for use in hydrodynamic simulation of high-pressure phenomena. Electronic properties are obtained from a modified Thomas–Fermi statistical model, while ion thermal motion is described by a multiphase equation of state combining Debye, Grüneisen, Lindemann, and fluid-scaling laws. The theory gives smooth and usable predictions for ionization state, pressure, energy, entropy, and Helmholtz free energy. When necessary, the results may be modified by a temperature-dependent pressure multiplier which greatly extends the class of materials that can be treated with reasonable accuracy. In this paper a comprehensive evaluation of the resulting thermodynamic data is given including comparison with other theories and shock-wave data.

Supported EOS Models
eostype(m) = 9, Stiff Gamma Law Equation of State

$$P + (\Gamma + 1)P_\infty = \frac{\Gamma}{V}(E + E_\infty), E + E_\infty = C_V T + P_\infty V$$

- Thermodynamically Consistent Stiff Gamma Law EOS
- Helmholtz free energy: $F = C_V T - C_V T \log[\Gamma C_V T V^\Gamma] - E_\infty + T S_\infty + P_\infty V$
  - Note: this is just the free energy for a perfect gas with a linear offset in specific entropy and specific volume
- P_∞= matdef(3,m), E_∞= matdef(10,m)
- Γ= matdef(16,m), C_V = matdef(30,m)
- Most often the default value for E_∞ = 0 is appropriate
- If the values for a reference temperature, specific volume, and pressure are known, an appropriate value for the specific heat at constant volume is

$$C_V = \frac{(P_0 + P_\infty)V_0}{\Gamma T_0}$$

Supported EOS Models
eostype(m) = 10, JWL EOS with temperature specified at a given density and energy

$$P = P_r(V) + \frac{w}{V}\left(E - E_r(V)\right), E - E_r(V) = C_V(T - T_r(V))$$

$$P_r(V) = Ae^{-R_1\frac{V}{V_0}} + Be^{-R_2\frac{V}{V0}}$$

$$E_r(V) = -\Delta E + \frac{AV_0}{R_1}e^{-R_1\frac{V}{V_0}} + \frac{BV_0}{R_2}e^{-R_2\frac{V}{V0}}$$

$$T_r(V) = T_0\left(\frac{V}{V_0}\right)^{-w}$$

- Note: For T_0=0 this recovers the standard JWL eos. Also a now zero value for T_0 may produce van der Waals loops for this model. For this model the reference pressure and energy are given by:

$$P_0 = P_r(V_0) = A + B, E_0 = E_r(V_0) = -\Delta E + \frac{AV_0}{R_1} + \frac{BV_0}{R_2}$$

Supported EOS Models
eostype(m) = 11: Steinberg-Mie-Grüneisen EOS:

- This is a variation of eostype(m) = 3 with temperature specified at a given density/energy:

$$P = P_r(V) + \frac{\Gamma(V)}{V}[E - E_r(V)], E - E_r(V) = C_V[T - T_r(V)]$$

$$C_V\left[\frac{d}{dV}T_r(V) + \frac{\Gamma(V)}{V}T_r(V)\right] = P_r(V) + E_r{}'(V), T_r(V_0) = T_0$$

$$P_r(V) = P_0 + \rho_0 c_0^2 \begin{cases} \dfrac{\eta}{[1-\eta s(\eta)]^2} & ,0 \le \eta \le 1 \\ \dfrac{[(1-\eta)^{-(\Gamma_0+1)} - 1]}{\Gamma_0 + 1} & ,\eta < 0 \end{cases}, \eta = \frac{V_0 - V}{V_0}, s(\eta) = s_1 + s_2\eta + s_3\eta^2$$

$$E_r(V) = E_0 + \begin{cases} \dfrac{P_r(V) + P_0}{2}(V_0 - V) & ,0 \le \eta \le 1 \\ \dfrac{c_0^2}{\Gamma_0 + 1}\left[\dfrac{(1-\eta)^{-\Gamma_0} - 1}{\Gamma_0} + \dfrac{\eta}{\Gamma_0 + 1}\right] & ,\eta < 0, P_r(V) = -E_r{}'(V) \end{cases}, \Gamma(V) = \begin{cases} \Gamma_0(1-\eta) + b\eta & ,0 \le \eta \le 1 \\ \Gamma_0 & ,\eta < 0 \end{cases}$$

- c_0=matdef(3,m), s_1=matdef(4,m), s_2=matdef(10,m), s_3= matdef(11,m)
- Γ_0=matdef(16,m), b = matdef(17.m), ρ_0= matdef(21,m), T_0= matdef(26,m), E_0= matdef(29,m)
- C_V=matdef(30,m), recommended value = $\frac{(P_0+P_\infty)V_0}{\Gamma_0 T_0}$
- For expansion $V > V_0$ this model is a stiff gamma law equation of state
- Parameter values from Steinberg, D.J., *Equation of State and Strength Properties of Selected Materials*, Lawrence Livermore National Laboratory, UCRL-MA-106439-rev. 1996. are appropriate
  - All quantities are dimensionlesss except for the reference sound speed, temperature, pressure, specific volume, and specific internal energy

Supported EOS Models
eostype(m) = 12, Linear density/pressure EOS

$$P = P_0 + \rho_0 c_0^2 \left(\frac{\rho}{\rho_0} - 1 \right)$$

$$E = E_0 + [\rho_0 c_0^2 - P_0][V - V_0] \text{-} \ c_0^2 \log \frac{V}{V_0} + C_V [T - T_0]$$

- P_0= matdef(3,m), E_0= matdef(4,m), $\rho_0 c_0^2$= matdef(16,m),
- ρ_0= matdef(21,m), T_0= matdef(26,m), C_V = matdef(30,m)

Supported EOS Models
eostype(m) = 13: JWL with automatically computed energy offset

$$P - P_s(V) = \frac{w}{V}\left(E - E_s(V)\right), E - E_s(V) = C_V\left(T - T_s(V)\right) + \Delta E, P_s(V) = Ae^{-R_1\frac{V}{V_0}} + Be^{-R_2\frac{V}{V_0}} + C\left(\frac{V}{V_0}\right)^{-(w+1)}$$

$$E_s(V) = V_0\left(\frac{A}{R_1}e^{-R_1\frac{V}{V_0}} + \frac{B}{R_2}e^{-R_2\frac{V}{V_0}} + \frac{C}{w}\left(\frac{V}{V_0}\right)^{-w}\right), T_s(V) = T_{ref}\left[\frac{\max\left(V, V_{CJ}\right)}{V_0}\right]^{-w} + \Delta T_{CJ}\min\left(0, \frac{V - V_{CJ}}{V_0}\right), T_0 = 298°K. P_0 = 1bar$$

$$\begin{cases} \frac{P_{CJ}}{1 - V_{CJ}} = R_1Ae^{-R_1\frac{V_{CJ}}{V_0}} + R_2Be^{-R_2\frac{V_{CJ}}{V_0}} + (1+w)\left(P_{CJ} - Ae^{-R_1\frac{V_{CJ}}{V_0}} - Be^{-R_2\frac{V_{CJ}}{V_0}}\right)\left(\frac{V_{CJ}}{V_0}\right)^{-1} & T_{CJ} > 0 \\ V_{CJ} = \frac{1}{2} & T_{CJ} \le 0 \end{cases}$$

$$C = \begin{cases} \left(P_{CJ} - Ae^{-R_1\frac{V_{CJ}}{V_0}} - Be^{-R_2\frac{V_{CJ}}{V_0}}\right)\left(\frac{V_{CJ}}{V_0}\right)^{w+1} & T_{CJ} > 0 \\ P_0 - Ae^{-R_1} - Be^{-R_2} & T_{CJ} \le 0 \end{cases}, \quad \Delta T_{CJ} = -wT_{ref}\left(\frac{V_{CJ}}{V_0}\right)^{-(w+1)}, \Delta E = \begin{cases} \frac{1}{2}\left(P_0 + P_{CJ}\right)\left(V_0 - V_{CJ}\right) - E_s\left(V_{CJ}\right) & T_{CJ} > 0 \\ -E_s(V_0) & T_{CJ} \le 0 \end{cases}$$

- Matdef(2,m):

Matdef(2,m)	Density	Pressure	Specific Internal Energy	Temperature
1	grams/cc	megabar	teraerg/gram	Kelvin
2	grams/cc	microbar	erg/gram	Kelvin
3	grams/cc	gigapascal	kilojoule/gram	Kelvin

- A = matdef(3,m), B = matdef(4,m), $C_V = \begin{cases} \text{matdef}(30, m) & T_{CJ} > 0 \\ \frac{V_{cold}}{w}\frac{P_0 - P_s(V_{cold})}{T_{cold} - T_s(V_{cold})} & T_{CJ} \le 0 \end{cases}$
- R_1 = matdef(10,m), R_2 = matdef(11,m), w = matdef(16,m), $\rho_0 = \frac{1}{V_0}$ = matdef(21,m)
- $\rho_{cold} = \frac{1}{V_{cold}}$ = matdef(33,m), T_{cold}= matdef(26,m), T_{CJ}= matdef(32,m), P_{CJ}= matdef(31,m)

Supported EOS Models
eostype(m) = 14, Davis Reactants Equation of State

$$P - P_s(V) = \frac{\Gamma(V)}{V}[E - E_s(V)]$$

$$P_s(V) = P_0 + \begin{cases} \hat{P}[\exp(4By) - 1] & ,V_0 < V \\ \hat{P}\left[\sum_{j=1}^{3} \frac{(4By)^j}{j!} + C\frac{(4By)^4}{4!} + \frac{y^2}{(1-y)^4}\right] & ,V < V_0 \end{cases}, y = 1 - \frac{V}{V_0}, \hat{P} = \rho_0 \frac{A^2}{4B}$$

$$E_s(V) = E_0 - \int_{V_0}^{V} P_s(v)dv\,, \Gamma(V) = \begin{cases} \Gamma_0 & ,V_0 < V \\ \Gamma_0 + Zy & ,V < V_0 \end{cases}$$

$$T(E,V) = T_s(V)\left\{\frac{1+\alpha_{st}}{C_V^0 T_s(V)}[E - E_s(V)] + 1\right\}^{\frac{1}{1+\alpha_{st}}}, T_s(V) = T_0 \exp(-Zy)\left(\frac{V}{V_0}\right)^{-(\Gamma_0+Z)}$$

- P_{scale} = matdef(2,m) (default 10^{10}= Gpa) – defines pressure scaling from μbar
- $e_{scale} = P_{scale}$, for fixed density units pressure and specific internal energy scale in the same way, from erg/gram
- ρ_0= matdef(3,m), E_0 = matdef(4,m) (e_{scale}), P_0 = matdef(5,m) (P_{scale})
- T_0 = matdef(6,m) (Kelvin), *A* = matdef(7,m), *B* = matdef(8,m)
- *C* = matdef(9,m), Γ_0 = matdef(10,m), Z = matdef(11,m), α_{st} = matdef(12,m)
- C_V^0 = matdef(13,m) (e_{scale}/Kelvin)

Supported EOS Models
eostype(m) = 15, Davis Products Equation of State

$$P - P_s(V) = \frac{\Gamma(V)}{\Gamma(V)}[E - E_s(V,\Delta E)], E - E_s(V,\Delta E) = C_V[T - T_s(V)]$$

$$P_s(V) = P_c\left(\frac{V}{V_c}\right)^{-k-a}\left[\frac{1}{2}\left(\frac{V}{V_c}\right)^{n} + \frac{1}{2}\left(\frac{V}{V_c}\right)^{-n}\right]^{\frac{a}{n}}\frac{k-1+F(V)}{k-1+a}, F(V) = \frac{2a\left(\frac{V}{V_c}\right)^{-n}}{\left[\left(\frac{V}{V_c}\right)^{n} + \left(\frac{V}{V_c}\right)^{-n}\right]}$$

$$E_s(V,\Delta E) = E_c\left(\frac{V}{V_c}\right)^{-k-a+1}\left[\frac{1}{2}\left(\frac{V}{V_c}\right)^{n} + \frac{1}{2}\left(\frac{V}{V_c}\right)^{-n}\right]^{\frac{a}{n}} + \Delta E, E_c = \frac{P_cV_c}{k-1+a}$$

$$-P_s'(V_{CJ}) = \frac{P_s(V_{CJ}) - P_0}{V_0 - V_{CJ}}, \Delta E = \frac{P_s(V_{CJ}) + P_s(V_{CJ})}{2} - (E_s(V,0) - E_0)$$

$$T_s(V) = T_c e^{\int_{V_c}^{V}\frac{\Gamma(v)}{v}dv}\left(\frac{V}{V_c}\right)^{-(k-1+a(1-b))}\left[\frac{1}{2}\left(\frac{V}{V_c}\right)^{n} + \frac{1}{2}\left(\frac{V}{V_c}\right)^{-n}\right]^{\frac{a}{n}(1-b)}, T_c = \frac{2^{-ab/n}}{k-1+a}\frac{P_cV_c}{C_V}$$

$$\Gamma(V) = k - 1 + (1-b)F(V), T'_s(V) + \frac{\Gamma(V)}{V}T_s(V) = 0$$

- P_{scale} = matdef(2,m) (default 10^{10}= Gpa) – defines pressure scaling from μbar
- $e_{scale} = P_{scale}$, for fixed density units pressure and specific internal energy scale in the same way,
- ρ_0= matdef(3,m), E_0 = matdef(4,m) (e_{scale}), P_0 = matdef(5,m) (P_{scale})
- V_c = matdef(6,m), P_c = matdef(7,m) (P_{scale}), T_c = matdef(8,m) ($Kelvin$)
- $a =$ matdef(9,m), $b =$ matdef(10,m), $n =$ matdef(11,m), $k =$ matdef(12,m)
- C_V= matdef(13,m) (e_{scale}/Kelvin)

Supported EOS Models eostype(m) = 16: Ideal Gas

- Ideal gas with the specific heat at constant pressure given as a polynomial in temperature. Two sets of coefficients for this polynomial are used, a high temperature and low temperature range.

$$PV = RT, \frac{C_p}{R} = \begin{cases} \sum_{i=1}^{5} a_i T^{i-1}, & T > T_s \\ \sum_{i=1}^{5} a_{i+7} T^{i-1}, & T < T_s \end{cases}, \frac{h}{RT} = \begin{cases} \frac{a_6}{T} + \sum_{i=1}^{5} \frac{a_i}{i} T^{i-1}, & T > T_s \\ \frac{a_{13}}{T} + \sum_{i=1}^{5} \frac{a_{i+7}}{i} T^{i-1}, & T < T_s \end{cases}$$

$$\frac{S}{R} = \begin{cases} a_1 \ln T + a_7 + \sum_{i=2}^{5} \frac{a_i}{i-1} T^{i-1}, & T > T_s \\ a_8 \ln T + a_{14} + \sum_{i=2}^{5} \frac{a_{i+7}}{i-1} T^{i-1}, & T < T_s \end{cases}$$

- Here *h* is the specific enthalpy, and the specific entropy is *S-RlogP*
- The above formulas hold for $T_{\min} \leq T \leq T_{\max}$, beyond these limits a constant specific heat a constant pressure is used
- $T_{\min}$=matdef(18,m), $T_{\max}$= matdef(19,m), T_s = matdef(20,m)
- *R* = matdef(30,m), a_i = matdef(3+*i*,m)